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Abstract

For a few particular waveguide problems, standard variational expressions have previously been shown to be upper or lower bounds on the quantities of interest. However, bounds have not previously been obtained for any truly three dimensional problem, that is, where the fields cannot be derived from a single scalar potential. An example is a three dimensional obstacle which contacts only one waveguide surface. As one consequence, no straightforward procedure exists for improving the approximations. Recently, Kato devised a rather general method for bounding the cotangent of the phase shift for a given angular momentum in a quantum mechanical central potential scattering problem. This method should be applicable whenever a system can be analyzed in terms of uncoupled standing waves each characterizable by one real phase shift. The method is here adapted to waveguides, including truly three dimensional problems. The obstacle must be symmetric about a plane perpendicular to the waveguide axis, with certain exceptions only one mode should propagate, and the system should be lossless. Analysis is then possible in terms of η_e and η_o , the real uncoupled phase shifts associated with the even and odd standing waves, respectively. The bounds obtained on $\cot\eta_e$ and $\cot\eta_o$ determine bounds on the equivalent network elements.

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1. Introduction

The introduction of variational techniques has greatly facilitated the solution of scattering problems in various fields. They were originally applied by Schwinger to scattering in an analysis of waveguide problems [1,2] and quantum mechanical problems [3] and, independently, by Hulthèn [4] in an analysis of quantum mechanical problems.[5] These techniques have subsequently proved to be useful in a wide variety of fields including optics, acoustics and water waves. Though they are clearly superior to previously-used techniques, variational techniques as applied to scattering theory suffer a major defect as compared to variational techniques as applied to the determination of point eigenvalues such as the resonant frequencies of vibrating systems or the bound state energy eigenvalues of quantum mechanical systems. This defect is that while the expressions are stationary, they are in general neither an upper nor a lower bound. Thus, given two different trial functions, one cannot generally know which of the two variational results is better; in particular, the incorporation of additional parameters in a given trial function does not guarantee a better result. Consequently, it would be desirable to be able to deduce bounds on the quantities of interest. Now, in fact in some particular waveguide preblems the variational expressions themselves have been shown to be upper or lower bounds.[1,2] These problems are not sufficiently general, however, to include all cases of practical interest. For example, no technique seems to have been devised which is capable of giving bounds on the relevant quantities for a truly three-dimensional case, that is, where the fields cannot be derived from a single scalar potential.

Now a rather general approach has been devised by T. Kato [6,7,8,9] for obtaining bounds on cot $(\eta - \theta)$, where η is the phase shift for a given angular momentum in a quantum mechanical central potential scattering problem and θ is a parameter chosen for convenience. This method should be applicable to any problem which can be analysed in terms of uncoupled standing waves each of which can be characterized by one real phase shift. It is the purpose of this paper to adapt the Kato formalism to scattering by obstacles in wave-guides, including the truly three dimensional problem. The problems to be considered, for reasons which will be discussed later, are subject to the following restrictions:

(1) The waveguide is uniform in the asymptotic region.

(2) Only the dominant mode propagates, with exceptions which will be mentioned later.

(3) The obstacle is symmetrical about a plane perpendicular to the axis of the waveguide.

(4) The waveguide and obstacle are lossless.

In the companion paper, [10] the Kato formalism is applied to some specific problems involving dielectric obstacles and it is found that with a simple trial function and a moderate amount of work one can obtain upper and lower bounds on cot $(\eta_o - \theta)$ and cot $(\eta_e - \theta)$ where η_e and η_o are the real uncoupled phase shifts associated with the even and odd standing waves, respectively. These bounds differ from one another by only a few per cent, even for obstacles whose dimensions are comparable with the transverse dimensions of the waveguide. In addition, for the obstacles considered, bounds can be obtained directly on the phase shifts themselves and on the elements of the equivalent 'T' network.

2. Applicability of the Kato method

Before proceeding to the waveguide case, it will be helpful to outline Kato's approach. A standard technique in the quantum theory of scattering of a particle by a central potential, $V(\underline{r}) = V(r)$, is to separate the wave into partial waves, i.e., the eigenfunctions of the angular momentum operator. For a specified angular momentum and energy, the effect of the potential on each incident partial wave is completely characterized by one real number, the phase shift. For the case of zero orbital angular momentum, which is the closest analogue to the waveguide case we are ultimately interested in, the phase shift η is determined by the equations

$$\mathcal{L}' u_\Theta = \left[\frac{d^2}{dr^2} + k^2 + W(r)\right] u_\Theta = 0 \quad , \quad 0 \leq r \leq \infty \tag{1a}$$

$$u_\Theta(0) = 0 \tag{1b}$$

$$u_\Theta(r) \to \cos(kr+\Theta) + \cot(\eta-\Theta)\sin(kr+\Theta) \quad , \; r \to \infty \tag{1c}$$

In the above expressions, k^2 and $W(r)$ are proportional to the total energy and the negative of the potential energy, respectively, and the normalization constant Θ satisfies $0 \leq \Theta < \pi$ but is otherwise arbitrary. The introduction of Θ provides an additional element of freedom.

Let $u_{\Theta t}$ be a trial wave function which satisfies the boundary condition (1b) and has the asymptotic form (1c) with a trial phase shift η_t, but which does not satisfy the wave equation (1a). (Trial quantities will be distinguished

from their exact counterparts by a subscript t.) From Green's theorem,

$$\int_0^\infty (u_\theta \mathcal{L}' u_{\theta t} - u_{\theta t} \mathcal{L}' u_\theta)\, dr = \left[u_\theta \frac{du_{\theta t}}{dr} - u_{\theta t} \frac{du_\theta}{dr} \right]_0^\infty \quad . \tag{2}$$

and the asymptotic forms of u_θ and $u_{\theta t}$, it follows that

$$k \cot(\eta - \theta) = k \cot(\eta_t - \theta) - \int u_{\theta t} \mathcal{L}' u_{\theta t} dr + \int w_\theta \mathcal{L}' w_\theta \, dr \quad , \tag{3}$$

where

$$w_\theta(r) \;=\; u_{\theta t}(r) - u_\theta(r) \quad . \tag{4}$$

Equation (3) is an identity. If $u_{\theta t}$ is a good approximation to u_θ, then w_θ is a small term of first order, and the error term $\int w_\theta \mathcal{L}' w_\theta \, dr$ is of second order. If the error term is neglected in equation (2), the remaining two terms on the right hand side can be evaluated explicitly and constitute a variational expression for $k \cot(\eta - \theta)$. (For certain values of θ, this expression reduces to previously known variational principles.)

Kato's major contribution was the determination of upper and lower bounds on the error term and, hence, on $k \cot(\eta - \theta)$.[6] Kato derives the inequality

$$- \alpha_\theta^{-1} \int \rho^{-1} (\mathcal{L}' u_{\theta t})^2 dr \leq \int w_\theta \mathcal{L}' w_\theta dr \leq \beta_\theta^{-1} \int \rho^{-1} (\mathcal{L}' u_{\theta t})^2 dr \tag{5}$$

where ρ is some non-negative weight factor to be chosen for convenience; α_Θ is the smallest positive eigenvalue and β_Θ the smallest (in absolute value) negative eigenvalue of the associated eigenvalue problem,

$$\mathcal{L}' \phi_n(r) + \mu_n \, \rho(r) \, \phi_n(r) = 0 \quad , \quad 0 \leq r \leq \infty \, . \tag{6}$$

The eigenfunctions ϕ_n and eigenvalues μ_n are determined by the boundary conditions that ϕ_n vanish at the origin and have the asymptotic phase shift, $\delta(\mu_n)$, given by

$$\delta(\mu_n) = \Theta + n\pi \quad , \quad n = 0, \pm 1, \ldots \qquad . \tag{7}$$

Even quite crude lower bounds on α_Θ and β_Θ in equation (5) will provide close bounds on the error term in equation (3) and, hence, on the phase shift, provided the error integral, $\int \rho^{-1}(\mathcal{L}' u_{\Theta t})^2 \, dr$, which vanishes for the exact wave function, can be made sufficiently small. Comparison potentials for which equation (6) can be solved exactly are employed in the estimation of α_Θ and β_Θ, together with a theorem which states that the phase shift increases monotonically with increasing 'potential', $W(r)$[6,7,8] (decreasing potential energy).

Let us now consider a one dimensional quantum mechanical scattering problem, which is a still closer analogue to the waveguide problem. This differs from the previous case in that the range of the independent variable extends from $-\infty$ to $+\infty$. The difference is fundamental, however, since there are now two channels, i.e., two sets of incoming and outgoing waves. In a scattering problem which contains n channels, the remote effects of the scattering

process are characterized by an n x n scattering matrix relating the amplitudes of the n outgoing waves to those of the n incoming waves. Since the n^2 elements of the scattering matrix are complex, there are $2n^2$ quantities in all. However, not all of these quantities are independent. It follows from conservation of probability (energy in the electromagnetic case) and time reversibility that the scattering matrix is unitary and symmetric, which reduces the number of independent quantities to $\frac{1}{2}n(n + 1)$.[11,12] In the case of scattering by a central potential, there is a channel corresponding to each value of the angular momentum, but since the potential does not couple the waves of different angular momentum there is a separate scattering problem for each channel characterized by a single number, the phase shift. In the one dimensional problem there are two channels; hence three independent quantities are required to characterize the scattering. For this case, the Kato method does not appear to be applicable. However, if we restrict ourselves to an even 'potential', $W(x) = W(-x)$, the number of independent parameters is reduced to two. Further, the two independent solutions of the wave equation can be taken as standing waves which are even and odd in x, each characterized by one real number, the phase shifts η_e and η_o, respectively. The even and odd solutions can be regarded as solutions to two completely independent scattering problems, distinguished by the boundary conditions. The odd solution is identical with the solution of the radial wave equation for zero angular momentum (an odd function vanishes at the origin) except that the integrals are multiplied by $\frac{1}{2}$ because the range of integration has been doubled. The Kato method can also be applied to the even solution with minor modifications. The details will not be presented here because of the close correspondence to the waveguide case which will now be treated.

In the waveguide problem two additional formal complications arise. Firstly, the problem is three dimensional so that the line integrals which appear in the variational principle are replaced by volume integrals. Secondly, the wave functions are vectors rather than scalars. It will be seen that these two complications do not cause any difficulty in principle; in particular, the assumed uniformity of the waveguide in the asymptotic region makes the problem effectively one dimensional in this region. However, there are two channels corresponding to each propagating mode. If the Kato method is to be applicable, then in line with the previous discussion the waveguide and obstacle must be such that it is possible to reduce the scattering problem to completely independent problems each characterized by one real number. The number of channels can be reduced to two by requiring that the waveguide have only one propagating mode, which is not a serious restriction in most applications. Then, as in the one dimensional case, the number of independent parameters can be reduced from three to two and the scattering problem to completely independent problems for even and odd solutions if the obstacle is symmetrical about a plane perpendicular to the axis of the waveguide.

More than one mode can be allowed to propagate if the obstacle is such that it does not couple these modes. As an example, consider a metallic or uniform dielectric obstacle in a rectangular waveguide in the form of a right circular cylinder parallel to the direction of polarization of the dominant mode, centered in the guide and extending between the conducting boundaries. It is possible to select the dimensions of the waveguide in such a way that in some range of frequencies there are only three propagating modes, usually designated TE_{10}, TE_{20} and TE_{01}.[12] These three modes are not coupled to one

another by such an obstacle, nor are the even and odd standing wave solutions corresponding to each mode coupled. Thus there is a total of six channels such that the scattering in each channel is a separate problem characterized by a single phase shift. A simpler example is that of a dielectric obstacle whose permittivity is an even function of the coordinate parallel to the axis of the waveguide only. The problem is then one dimensional and we can consider an arbitrary number of propagating modes. for the various channels are uncoupled and each is characterized by a single phase shift. The problem of multiple propagating modes will not be considered further. It will henceforth always be understood that just the dominant mode propagates.

In some cases the symmetry of the obstacle is such that the scattering can be described in terms of a scalar wave function rather than a vector wave function, which may result in considerable simplification. For example, in a rectangular waveguide the dominant mode can be described variously as a TE wave propagating parallel to the axis of the waveguide, as a TM wave propagating parallel to the axis of polarization, or as a TE wave propagating in a direction perpendicular to both of these axes. Any finite obstacle destroys uniformity in the direction of the waveguide, but it may possess sufficient symmetry to preserve uniformity in one of the perpendicular directions, in which case the TE or TM description still applies. Now TE and TM waves can be derived from Hertzian electric and magnetic vector potentials, respectively, which are parallel to the propagation direction of the TE and TM waves respectively. Thus the fields are characterized by a single scalar function, the component along the appropriate axis of propagation of the Hertzian vector potential.

If the symmetry of the obstacle permits description of the fields in terms of a TM wave propagating parallel to the axis of polarization, the electric field is proportional to the vector potential, and the vector equations derived below go over to scalar equations directly. For the symmetry which permits description in terms of a TE wave, there is no such simple correspondence and the scalar formulation of the problem requires a separate derivation starting directly from the Hertzian vector potential formulation. Only the vector formulation will be presented here, though in the TE case it might be simpler to use the scalar formulation.

3. Variational principles for waveguides

In this section we shall derive the variational principle for a waveguide for both metallic and dielectric obstacles, with the four restrictions noted in the Introduction. In line with the previous discussion, it then follows that the general scattering problem reduces to two independent scattering problems, each of which can be characterized by just one real phase shift.

Assuming a time dependence $\exp(-i\omega t)$, the electric field intensity, $\underline{E}(\underline{r})$, satisfies the equations

$$\mathcal{L}\underline{E} = -\underline{\nabla} \times \underline{\nabla} \times \underline{E} + (\omega^2/c^2 + W)\underline{E} = 0 \tag{8a}$$

$$\underline{\nabla} \cdot \underline{E} = 0 \tag{8b}$$

where c is the velocity of light, ϵ is the relative permittivity, and where the 'potential' W is defined by $W = \omega^2(\epsilon - 1)/c^2$; the quantum mechanical analogue of W is proportional to the negative of the potential. In addition, $\underline{E}$ is required to be normal to all conducting surfaces including any metallic obstacles.

Let the z-coordinate be parallel to the axis of the waveguide. It follows from restriction (3) that $W(z) = W(-z)$, and the general solution can be expressed as a linear combination of standing wave solutions which are even and odd functions of z. In what follows, subscripts e and o will be used to denote quantities associated with the even and odd functions respectively, but will be omitted wherever the formalism is the same for both functions. The solutions are required to have the asymptotic forms for $z \to +\infty$

$$\underline{E}_{\theta e}(\underline{r}) = \underline{e}(x,y)\ \left|-\sin(kz+\theta) + \cot(\eta_e - \theta)\ \cos(kz+\theta)\right| \tag{9a}$$

$$\underline{E}_{\theta o}(\underline{r}) = \underline{e}(x,y)\ \left|\ \cos(kz+\theta) + \cot(\eta_o - \theta)\ \sin(kz+\theta)\right| \tag{9b}$$

where $\underline{e}(x,y)$ is the form function for the dominant mode and where θ satisfies $0 \leq \theta < \pi$. The utility of the parameter θ will become apparent as we go along.

The trial functions are distinguished from the exact functions by the subscript t, and are required to be even and odd and to have the asymptotic forms given by equations (9) except for the substitution of trial phase shifts η_{et} and η_{ot} for the exact phase shifts η_e and η_o. In addition, the trial function is required to be normal to all conducting surfaces and both the function and first derivatives are required to be continuous in the interior of the waveguide.

Consider the integral

$$\int (\underline{E}\cdot\mathcal{L}\ \underline{E}_t - \underline{E}_t \cdot \mathcal{L}\ \underline{E})d\tau = -\int (\underline{E} \cdot \underline{\nabla} \times \underline{\nabla} \times \underline{E}_t - \underline{E}_t \cdot \underline{\nabla} \times \underline{\nabla} \times \underline{E})d\tau \tag{10}$$

where the range of integration is over the interior of the waveguide. (It is to be understood, from here on, that 'the interior of the waveguides' excludes any metallic obstacles.) The second term in the integrand on the left hand side of equation (10) vanishes by virtue of equation (8a), and the right hand side can be transformed by Green's theorem to give

$$\int \underset{\sim}{E} \cdot \mathcal{L} \, \underset{\sim}{E}_t d\tau = \int (\underset{\sim}{E} \times \underset{\sim}{\nabla} \times \underset{\sim}{E}_t - \underset{\sim}{E}_t \times \underset{\sim}{\nabla} \times \underset{\sim}{E}) \cdot d\underset{\sim}{\sigma} \quad . \tag{11}$$

The surface integral vanishes on the conducting surfaces since $\underset{\sim}{E}$ and $\underset{\sim}{E}_t$ are required to be normal to these surfaces, and the contribution from the asymptotic region is

$$\int \underset{\sim}{E}_\Theta \cdot \mathcal{L} \, \underset{\sim}{E}_{\Theta t} d\tau = 2k \left[\cot(\eta_t - \Theta) - \cot(\eta - \Theta) \right] \int \left[\underset{\sim}{e}(x,y) \times \underset{\sim}{a}_z \right]^2 d\sigma \tag{12}$$

where $\underset{\sim}{a}_z$ is the unit vector in the z direction and the surface integral is over the cross section of the wave guide. It is convenient at this point to adopt a normalization and notation conforming more closely to that of Kato.[6] Let $\underset{\sim}{u}_\Theta$ and $\underset{\sim}{w}_\Theta$ be defined by

$$\underset{\sim}{u}_\Theta \equiv \left\{ \int \left[\underset{\sim}{e}(x,y) \times \underset{\sim}{a}_z \right]^2 d\sigma \right\}^{-\frac{1}{2}} \underset{\sim}{E}_\Theta \tag{13a}$$

$$\underset{\sim}{w}_\Theta = \underset{\sim}{u}_{\Theta t} - \underset{\sim}{u}_\Theta \tag{13b}$$

With these definitions, equation (12) can be written as

$$k\cot(\eta-\theta) = k\cot(\eta_t-\theta) - \frac{1}{2}\int \underset{\sim}{u}_{\theta t}\cdot \mathcal{L}\, \underset{\sim}{u}_{\theta t}\, d\tau + \frac{1}{2}\int \underset{\sim}{w}_{\theta}\cdot \mathcal{L}\, \underset{\sim}{w}_{\theta}\, d\tau \qquad (14)$$

in analogy with equation (3). The factor $\frac{1}{2}$ arises because the range of integration has been doubled. The first two terms on the right hand side of equation (14) can be calculated by specifying the trial function, and constitute a variational approximation for $k\cot(\eta-\theta)$. The third term, $\frac{1}{2}\int \underset{\sim}{w}_{\theta}\cdot \mathcal{L}\, \underset{\sim}{w}_{\theta}\, d\tau$, is the error term and is of the order of the square of the error in the trial function.

We now derive one consequence of equation (14). We have η as the phase shift associated with W. We let $\eta + d\eta$ be the phase shift associated with W + dW. where $dW(r) \geq 0$ for all r. Applying equation (14) to the determination of $\eta + d\eta$, we choose for our trial function the <u>exact</u> solution $\underset{\sim}{u}_{\theta}$ associated with W. We find

$$d\eta = (\tfrac{1}{2}\sin^2\eta/k) \int u_{\theta}^{2}(r)\; dW(r)\; dr \geq 0 \quad .$$

where the inequality is a consequence of the non-negativeness of $dW(r)$ and the reality of $\underset{\sim}{u}_{\theta}(r)$. More generally, it then follows that if $W_2(r) \geq W_1(r)$, then $\eta_2 \geq \eta_1$. This result is generally referred to as the monotonicity theorem.

4. Rigorous bounds on the error

Kato's method for obtaining rigorous bounds on the error term, and hence on $\cot(\eta-\theta)$, can be applied to the waveguide case with minor modification. In order to accomplish this, we make use of the following information about $\underset{\sim}{w}_\theta$:

$$\mathcal{L}\underset{\sim}{w}_\theta = \mathcal{L}\underset{\sim}{u}_{\theta t} \tag{15a}$$

$$\underset{\sim}{w}_{\theta e} \rightarrow C_e' \, \underset{\sim}{e}(x,y)\cos(kz+\theta) \quad , \quad z \rightarrow +\infty \tag{15b}$$

$$\underset{\sim}{w}_{\theta o} \rightarrow C_o' \, \underset{\sim}{e}(x,y)\sin(kz+\theta) \quad , \quad z \rightarrow +\infty \tag{15c}$$

where C_e' and C_o' are unknown constants. Also, $\underset{\sim}{w}_{\theta e}$ and $\underset{\sim}{w}_{\theta o}$ are even and odd functions of z respectively; $\underset{\sim}{w}_\theta$ is normal to all conducting surfaces, and $\underset{\sim}{w}_\theta$ and its first derivatives are continuous in the interior of the waveguide. Consider the equation

$$\mathcal{L}\underset{\sim}{\phi}(\underset{\sim}{r}) + \mu\rho(\underset{\sim}{r})\underset{\sim}{\phi}(\underset{\sim}{r}) = 0 \tag{16}$$

The function $\underset{\sim}{\phi}(\underset{\sim}{r})$ is required to be normal to all conducting surfaces. The weight function $\rho(\underset{\sim}{r}) \geq 0$ is an even function of z and tends to zero at large distances from the obstacle in such a way that $\int \rho(\underset{\sim}{r})d\tau$ converges. Equation (16) may be regarded as a scattering problem of the type of equation (8), with a 'potential' $W + \mu\rho$. The even and odd standing wave solutions are associated with entirely separate problems and the distinction between them is not relevant to the following discussion. Let $\delta(\mu)$ be the phase shift corresponding to this 'potential'. (The choice of ρ must be such that this problem also

satisfies the four restrictions listed in the introduction in order that there be just one phase shift $\delta(\mu)$ associated with each value of μ.) Equation (16) will be referred to as the associated eigenvalue problem with eigenvalues μ_n and eigen functions $\underset{\sim}{\phi}_n(\underset{\sim}{r})$ when $\delta(\mu_n)$ is restricted by the condition

$$\delta(\mu_n) = \theta + n\pi \quad . \tag{17}$$

If $\underset{\sim}{f}$ and $\underset{\sim}{g}$ are two functions which satisfy the boundary conditions appropriate to $\underset{\sim}{\phi}_n$, then it follows from Green's theorem that

$$\int \underset{\sim}{f} \cdot \mathcal{L}\, \underset{\sim}{g}\, d\tau = \int \underset{\sim}{g} \cdot \mathcal{L}\, \underset{\sim}{f}\, d\tau \tag{18}$$

where the integrals are over the interior of the waveguide. Thus the operator $\mathcal{L}$ restricted by these boundary conditions is hermitean; it follows that the eigenvalues are real and the eigenfunctions satisfy orthogonality relations

$$k \int \underset{\sim}{\phi}_m \cdot \underset{\sim}{\phi}_n \rho \, d\tau = \delta_{mn} \tag{19}$$

where $\delta_{mn} = 1$ if $m = n$ and $\delta_{mn} = 0$ if $m \neq n$ and the normalization is chosen for convenience.

Using the monotonicity theorem discussed earlier, it follows since $\rho(r) \geq 0$ for all r that

$$\frac{d\delta(\mu)}{d\mu} \geq 0 \ . \tag{20}$$

The eigenvalues therefore satisfy the relationship

$$\mu_{n+1} \geq \mu_n \quad . \tag{21}$$

It can be shown that the eigenfunctions $\underset{\sim}{\phi}_n$ form a complete set in the sense that the Parseval identities hold for any functions $\underset{\sim}{F}$, $\underset{\sim}{G}$ which satisfy certain symmetry conditions to be discussed in the following section, which are normal to all conducting surfaces and which are continuous and have continuous first derivatives, that is

$$k \int F^2 \rho \, d\tau = \sum a_n^{\,2} \quad , \quad k \int \underset{\sim}{F} \cdot \underset{\sim}{G} \rho \, d\tau = \sum a_n b_n \quad ,$$

$$k \int G^2 \rho \, d\tau = \sum \, b_n^{\,2} \quad : \tag{22}$$

the a_n and b_n are Fourier coefficients defined by

$$a_n = k \int \underset{\sim}{\phi}_n \cdot \underset{\sim}{F} \rho \, d\tau \quad , \quad b_n = k \int \underset{\sim}{\phi}_n \cdot \underset{\sim}{G} \rho \, d\tau \quad . \tag{23}$$

Now let $\underset{\sim}{F}$ satisfy the boundary conditions (17) and set $\underset{\sim}{G} = \rho^{-1} \mathcal{L} F$. Then

$$b_n = k \int \underset{\sim}{\phi}_n \cdot \mathcal{L} \underset{\sim}{F} \, d\tau = k \int \mathcal{L} \underset{\sim}{\phi}_n \cdot \underset{\sim}{F} \, d\tau = - \mu_n k \int \underset{\sim}{\phi}_n \cdot \underset{\sim}{F} \rho \, d\tau$$

$$= - \mu_n a_n \tag{24}$$

where we have made use of the hermitean property of $\mathcal{L}$. equation (18).

The Parseval identities become

$$k \int F^2 \rho d\tau = \sum \mu_n^{-2} b_n^2 \qquad (25a)$$

$$k \int \underset{\sim}{F} \cdot \mathcal{L} \underset{\sim}{F} d\tau = -\sum \mu_n^{-1} b_n^2 \qquad (25b)$$

$$k \int (\mathcal{L} \underset{\sim}{F})^2 \rho^{-1} d\tau = \sum b_n^2 \quad . \qquad (25c)$$

Let α_Θ be the smallest positive eigenvalue and $-\beta_\Theta$ the smallest (in absolute value) negative eigenvalue, so that $-\alpha_\Theta^{-1} \leq -\mu_n^{-1} \leq \beta_\Theta^{-1}$. Then it follows from equations (25) that

$$-\alpha_\Theta^{-1} \int (\mathcal{L} \underset{\sim}{F})^2 \rho^{-1} d\tau \leqq \int \underset{\sim}{F} \cdot \mathcal{L} \underset{\sim}{F} d\tau \leqq \beta_\Theta^{-1} \int (\mathcal{L} \underset{\sim}{F})^2 \rho^{-1} d\tau \quad . \qquad (26)$$

The point is that while $\mathcal{L}$ is an unbounded operator, $\mathcal{L}^{-1}$ is a bounded operator, its eigenvalues ranging from $-\beta_\Theta^{-1}$ to α_Θ^{-1}. If we identify $\underset{\sim}{F}$ with $\underset{\sim}{w}_\Theta$ defined by equation (13b) and recognize that $\mathcal{L} \underset{\sim}{w}_\Theta = \mathcal{L} \underset{\sim}{u}_{\Theta t}$, equation (26) implies that

$$-\tfrac{1}{2} \alpha_\Theta^{-1} \int (\mathcal{L} \underset{\sim}{u}_{\Theta t})^2 \rho^{-1} d\tau \leq \tfrac{1}{2} \int \underset{\sim}{w}_\Theta \cdot \mathcal{L} \underset{\sim}{w}_\Theta d\tau \leq \tfrac{1}{2} \beta_\Theta^{-1} \int (\mathcal{L} \underset{\sim}{u}_{\Theta t})^2 \rho^{-1} d\tau \ . \quad (27)$$

The quantity $\tfrac{1}{2} \int (\mathcal{L} \underset{\sim}{u}_{\Theta t})^2 \rho^{-1} d\tau$ is determined by specifying the trial function $\underset{\sim}{u}_{\Theta t}$. Thus the problem of obtaining rigorous upper and lower bounds on the error term in equation (14) is reduced to that of obtaining rigorous lower bounds on α_Θ and β_Θ. If the trial function $\underset{\sim}{u}_{\Theta t}$ is a good approximation

to the exact function $\underline{u}_\theta$, $(\mathcal{L}\, \underline{u}_{\theta t})^2$ is a small term of second order, and even crude lower bounds on α_θ and β_θ can provide close bounds on the error term and hence on $\cot(\eta-\theta)$.

5. Completeness

The question of completeness is rather more complicated for the present waveguide case than for the one independent variable quantum mechanical case discussed by Kato. In particular, it will be shown that the $\underline{\phi}_n$ as defined by the differential equation, (16), and by the boundary condition, equation (17), are not necessarily complete. Limitations are thereby imposed on the trial function, in addition to the boundary conditions stated in Section 3, if the bounds deduced in Section 4 on $\cot(\eta-\theta)$ are to be valid. It will be seen, however, that the limitations are in no sense severe; on the contrary, it will only be required that the trial function have the same symmetry properties as the true function. Clearly, no restrictions whatever are thereby introduced on the accuracy of the bounds that can be achieved. The fact remains that each of the symmetry properties must be recognized if the Kato bounds are to be valid.

That the $\underline{\phi}_n$ are not always complete can be seen by considering the simple example of a waveguide for which the obstacle is a dielectric slab which extends to the conducting boundaries of the waveguide and whose permittivity is independent of x and y. Then each of the $\underline{\phi}_n$ will everywhere (not only asymptotically) have the same x and y dependence. In particular, each $\underline{\phi}_n$ can be expressed as a product of $\underline{e}(x,y)$ and a function of z, where $\underline{e}(x,y)$ is the form function appropriate to the dominant mode, and the problem is then effectively one dimensional. In this example the $\underline{\phi}_n$ are obviously not a complete set; this need cause no concern, however. It is clear that the true

solution $\underset{\sim}{u}$ would also have the same x,y dependence as the dominant mode. One would then choose the trial function $\underset{\sim}{u}_t$ to have this x,y dependence, in which case $\underset{\sim}{w} = \underset{\sim}{u}_t - \underset{\sim}{u}$ would also have this x,y dependence, and this $\underset{\sim}{w}$ could be expanded in terms of the $\underset{\sim}{\phi}_n$. On the other hand, if one failed to recognize the one dimensionality of the problem and used any x,y dependence other than that given by $\underset{\sim}{e}(x,y)$, $\underset{\sim}{w}$ could not be expanded in terms of the $\underset{\sim}{\phi}_n$ and the bounds obtained on $\cot(\eta-\theta)$ in Section 4 would not be rigorous.

In discussing the question of completeness for an arbitrary $W(x,y,z)$, it is assumed for simplicity of presentation that W and ρ both vanish identically beyond $|z| = d$. It is believed, however, that the conclusions of this section can be established under more general circumstances. Now it can be shown that the eigenfunctions of a positive definite, hermitian operator form a complete set.[13] Actually, the essential point is not that the operator be positive definite but rather that there be a minimum negative eigenvalue. That there is a minimum negative eigenvalue in the associated eigenvalue problem follows from the assumption that W and ρ vanish identically beyond $|z| = d$, since there is a minimum number of nodes which the wave functions can have in the region $-d < z < d$.

It remains to determine the boundary conditions for which $\mathcal{L}$ is hermitian. It follows from Green's theorem that for two functions $\underset{\sim}{f}(\underset{\sim}{r})$ and $\underset{\sim}{g}(\underset{\sim}{r})$ which are continuous and have continuous first derivatives, and which are normal to the conducting boundaries of the waveguide,

$$\int (\underset{\sim}{f} \cdot \mathcal{L}\, \underset{\sim}{g} - \underset{\sim}{g} \cdot \mathcal{L}\, \underset{\sim}{f})d\tau = \int (\underset{\sim}{f} \times \underset{\sim}{\nabla} \times \underset{\sim}{g} - \underset{\sim}{g} \times \underset{\sim}{\nabla} \times \underset{\sim}{f}) \cdot d\underset{\sim}{\sigma}$$

where the surface integral is over end surfaces of the waveguide in the asymptotic region. Consider a set of eigenfunctions $\underset{\sim}{\psi}_m$ of the differential

equation

$$\mathcal{L}\,\underset{\sim}{\psi}_m + \lambda_m\,\rho\,\underset{\sim}{\psi}_m = 0 \quad ,$$

defined by the boundary condition

$$\int \left(\underset{\sim}{\psi}_m \times \underset{\sim}{\nabla} \times \underset{\sim}{\psi}_n - \underset{\sim}{\psi}_n \times \underset{\sim}{\nabla} \times \underset{\sim}{\psi}_m \right) \cdot d\underset{\sim}{\sigma} = 0$$

for all m and n. Then the operator $\mathcal{L}$ is hermitian with respect to the set of functions $\underset{\sim}{\psi}_m$ and it follows that these functions form a complete set. The set of functions $\underset{\sim}{\psi}_m$ can be divided into two subsets. The first subset consists of functions which have the asymptotic form of the dominant mode and whose phase shifts $\delta(\lambda_m)$ differ by integral multiples of π. This subset is identical with a set of associated eigenfunctions $\underset{\sim}{\phi}_n$ with $\lambda_m = \mu_n$. The second subset consists of functions which vanish asymptotically. These functions do not occur in the one independent variable quantum mechanical problem with fixed, positive energy, and it follows that for that problem each of the $\underset{\sim}{\psi}_m$ equals one of the $\underset{\sim}{\phi}_n$ which then form a complete set. However, in the waveguide problem the functions which vanish asymptotically can exist under special circumstances which will now be considered.

In the region of large $|z|$, where W and ρ are zero, each $\underset{\sim}{\psi}_m$ is a superposition of evanescent waveguide modes and of the dominant waveguide mode. (The term waveguide mode will be used for modes in the absence of an obstacle.) The coefficient of the dominant waveguide mode will be denoted by C_m. There are two alternative possibilities.

(1) If each C_m is different from zero, each $\underset{\sim}{\psi}_m$ equals one of the $\underset{\sim}{\phi}_n$ and each λ_m equals one of the μ_n. The $\underset{\sim}{\phi}_n$ then form a complete set.

(2) If $C_m = 0$ for any m, the corresponding $\underset{\sim}{\psi}_m$ vanishes asymptotically and the $\underset{\sim}{\phi}_n$ do not then form a complete set.

The condition $C_m = 0$ can only arise if some of the evanescent waveguide modes are not coupled to the dominant waveguide mode. This lack of coupling can only occur if W and ρ have some special symmetry property. We have already given one example in which W and ρ are independent of the transverse coordinates. As another example, we consider a rectangular waveguide where the z axis is the axis of the waveguide, the y axis is the axis of polarization of the dominant mode and the waveguide extends from $x = 0$ to $x = a$. We further specify that W and ρ are independent of y and are even functions of $x - \frac{1}{2}a$. Then the functions $\underset{\sim}{\phi}_n$ share the polarization of the dominant mode, are independent of y, and are even functions of $x - \frac{1}{2}a$; the $\underset{\sim}{\phi}_n$ are not, therefore, a complete set. The set of functions $\underset{\sim}{\psi}_m$ which is complete includes functions which are odd functions of $x - \frac{1}{2}a$, functions which depend upon y and whose polarization is not along the y axis, and functions with both of these properties, all of which vanish asymptotically. However, the exact solution $\underset{\sim}{u}$ is also polarized parallel to the y axis, is independent of y, and is an even function of $x - \frac{1}{2}a$. If the trial function $\underset{\sim}{u}_t$ is chosen to have the same properties it will be possible to expand $\underset{\sim}{w}$ in terms of the incomplete set $\underset{\sim}{\phi}_n$.

In summary, if W and ρ have no symmetry properties, the $\underset{\sim}{\psi}_m$ are identical with the $\underset{\sim}{\phi}_n$ so the latter form a complete set. On the other hand, if W and ρ do have some symmetry properties, the functions $\underset{\sim}{\phi}_n$ have some common symmetry properties and do not then form a complete set. The set of functions $\underset{\sim}{\psi}_m$ is complete, however, since it then contains functions which vanish asymptotically and have different symmetry properties. For an arbitrary trial function $\underset{\sim}{u}_t$ the difference function $\underset{\sim}{w}$ could only be expanded in terms of the $\underset{\sim}{\psi}_m$;

one could not then use the monotonicity theorem to order the eigenvalues in terms of the phase shifts, an ordering which is essential for the applicability of the method used in the following section for the determination of bounds on α_Θ and β_Θ. It is of course quite possible that methods could be devised for the determination of bounds on α_Θ and β_Θ even for the case for which evanescent modes must be included; if, however, $\underline{u}_t$ is chosen with the correct symmetry, $\underline{w}$ can be expanded in terms of the $\underline{\phi}_n$ and the question does not then arise.[14]

6. Lower bounds on α_Θ and β_Θ

The general procedure for obtaining lower bounds on α_Θ and β_Θ involves the use of comparison potentials for which the scattering problem can be solved exactly, and the monotonicity theorem, equation (20). A number of cases have been treated in the literature.[6,7] In this section, we will consider just three special cases applicable to a wide variety of waveguide scattering problems. We restrict ourselves to waveguides which are of uniform cross-section everywhere. These three cases are particularly simple to apply.

In the context of the following discussion, metallic obstacles may be regarded as dielectric obstacles with infinite negative permittivity. (This comment does not apply to the preceding discussion of the variational principle and associated eigenvalue because the integrals would be divergent with an infinite 'potential'.) Suppose the obstacle does not extend beyond $z = \pm d$, and that ρ is identically zero for $|z| > d$ and positive for $|z| < d$.

We will first obtain a lower bound on β_Θ. As μ approaches $-\infty$, it is

evident that the phase shift $\delta(\mu)$ of the associated eigenvalue problem approaches -kd in the odd case and $-kd - \frac{1}{2}\pi$ in the even case. Now if $-kd > \Theta - \pi$ in the odd case or $-kd - \frac{1}{2}\pi > \Theta - \pi$ in the even case and if $\eta < \Theta$, then as shown in Figure 1, there can be no negative eigenvalues and β_Θ can be regarded as infinite. In this case the error term in equation (14) is always negative, and the variational approximation to $k \cot(\eta-\Theta)$ is always an upper bound on the exact value.

A lower bound on α_Θ can be obtained as follows. We know from the monotonicity theorem, equation (20), that the phase shift $\delta(\mu)$ is less than the phase shift $\delta'(\mu)$ which would result if the obstacle were replaced by a dielectric slab which fills the space $-d < z < d$ out to the conducting boundaries of the waveguide, and whose 'potential' is equal to the maximum value of $W + \mu\rho$. This phase shift is given by

$$\delta'_e(\mu) = -kd + \tan^{-1}\left(\frac{k'd}{kd} \tan k'd\right) \qquad (28a)$$

$$\delta'_o(\mu) = -kd + \tan^{-1}\left(\frac{kd}{k'd} \tan k'd\right) \qquad (28b)$$

$$k' = k'(\mu) = \left[k^2 + (W + \mu\rho)_{max}\right]^{\frac{1}{2}} \qquad (28c)$$

It can be seen from Figure 2 that a useful lower bound on α_Θ is provided by the value of μ, to be denoted by α_Θ', defined by $\delta'(\alpha_\Theta') \equiv \Theta$, provided that $\eta' \equiv \delta'(0) < \Theta$ and $\eta > \Theta - \pi$. For a dielectric obstacle η will always be greater than zero and the last condition will automatically be satisfied.

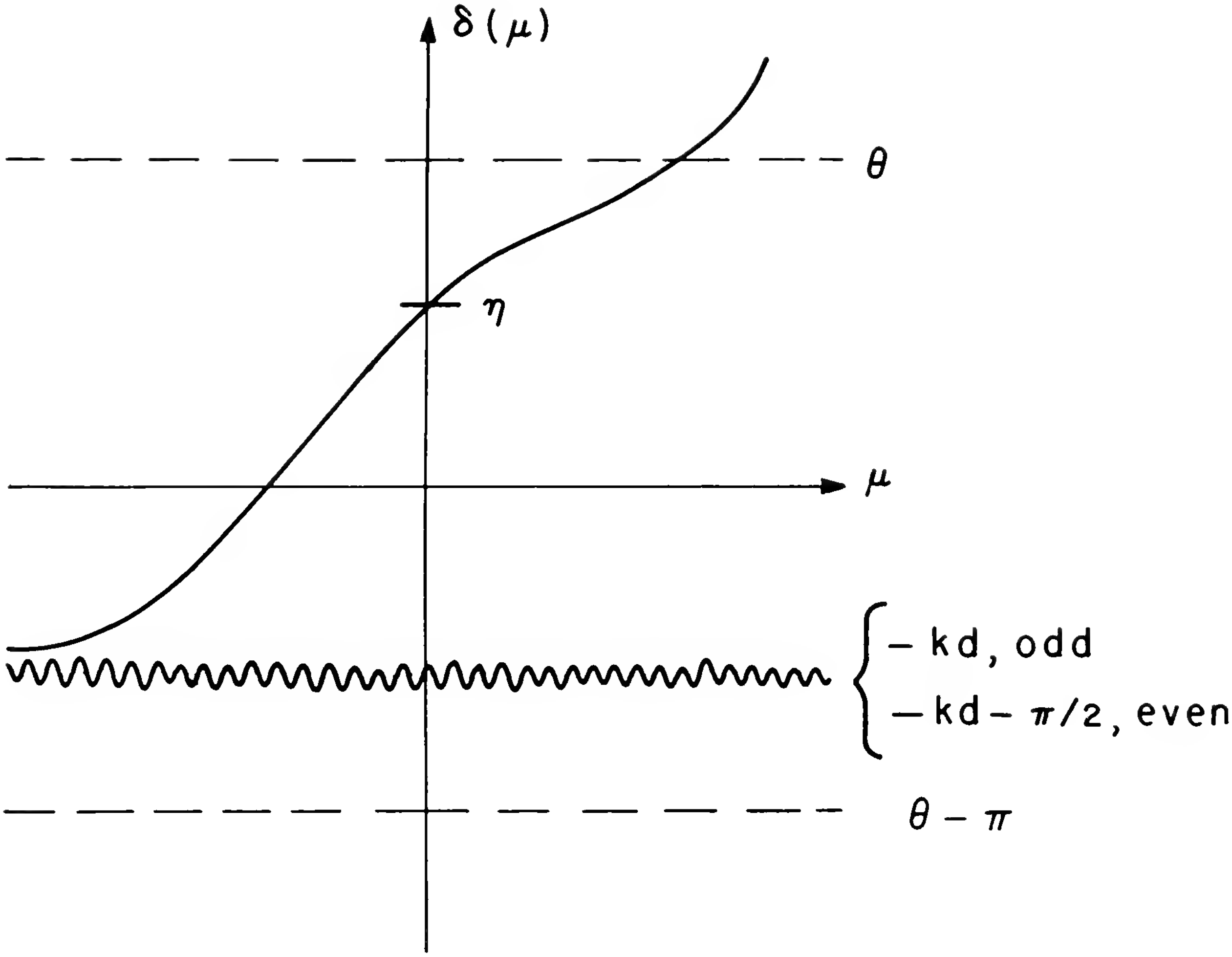

Figure 1

Determination of a lower bound on β_Θ assuming $\eta < \Theta$, and assuming $-kd > \Theta - \pi$ in the odd case and $-kd - \frac{1}{2}\pi > \Theta - \pi$ in the even case. Since $\delta(\mu)$ must exceed $\Theta - \pi$, β_Θ is infinite.

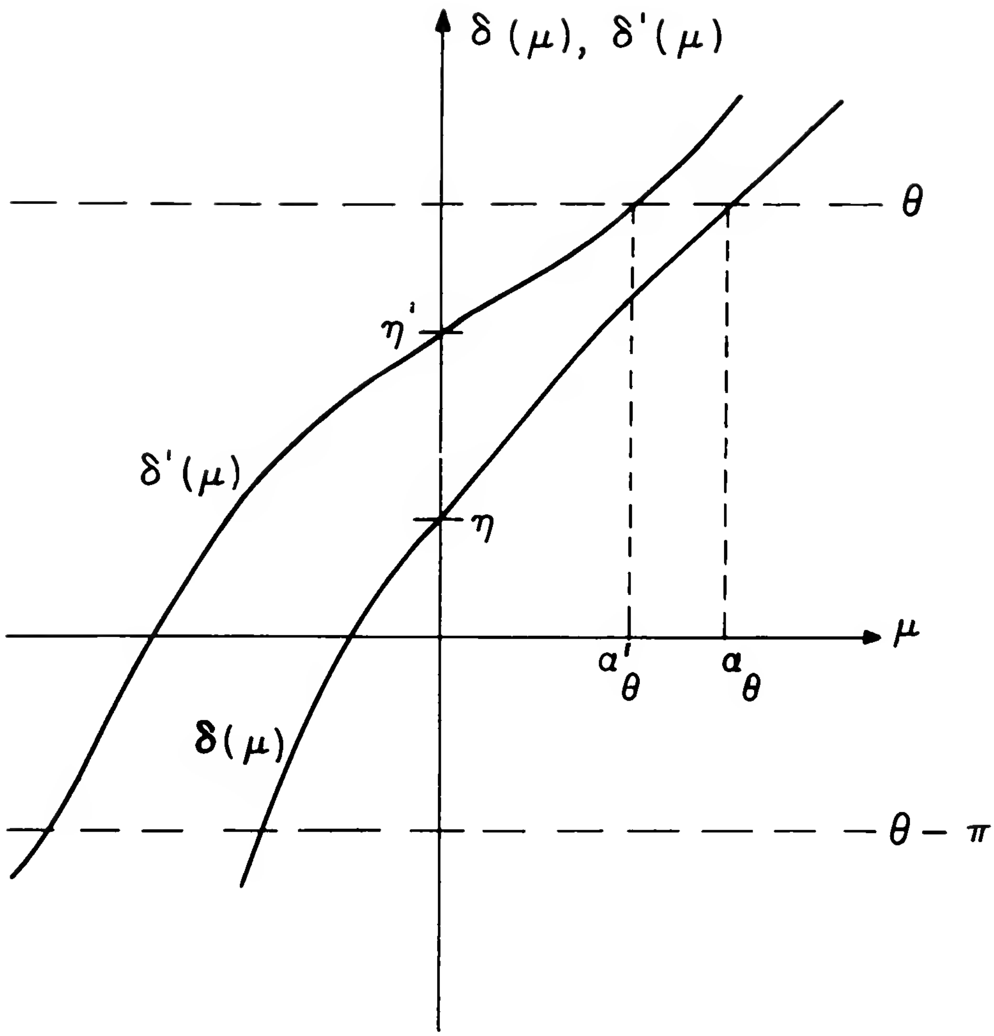

Figure 2

Determination of a lower bound on α_θ assuming $\eta' < \theta$ and $\eta > \theta - \pi$. The upper curve corresponds to a dielectric slab filling the guide in the range $-d < z < d$, whose 'potential' equals the maximum 'potential' of the obstacle. From the monotonicity theorem, $\delta'(\mu) > \delta(\mu)$ and therefore $\alpha_\theta' < \alpha_\theta$.

From the rough bounds already obtained on η,

$$-kd - \tfrac{1}{2}\pi < \eta_e < \eta_e' \qquad (29a)$$

$$-kd < \eta_o < \eta_o' \qquad (29b)$$

it follows that a sufficient condition for obtaining lower bounds on α_Θ and β_Θ by the procedure described above is that $d(k^2 + W_{max})^{\frac{1}{2}}$ be less than $\frac{1}{2}\pi$ in the even case and less than π in the odd case. An equivalent statement is that 2d must be less than $\frac{1}{2}\lambda$ in the even case and λ in the odd case, where λ is the smallest guide wavelength in the dielectric. However, it should be noted that these restrictions are by no means fundamental, since there are many more possibilities for obtaining lower bounds on α_Θ and β_Θ.

There is one case of interest in which β_Θ can be determined exactly.[6] If W is everywhere positive we can choose $\rho = W$. Then the 'potential' of the associated eigenvalue, $W + \mu\rho$, vanishes when $\mu = -1$ and the phase shift $\delta(-1)$ vanishes also. If we choose $\Theta = 0$, it is evident that $\mu = -1$ is an eigenvalue. Furthermore, if we know that $\eta < \pi$, it is the smallest (in absolute value) negative eigenvalue as can be seen from Figure 3. Thus for the case in which $W > 0$, $\rho = W$, $\Theta = 0$ and $\eta < \pi$, the eigenvalue β_o is given exactly by

$$\beta_o = 1 \qquad (30)$$

(More generally, if $W > 0$, if $\rho = W$, and if $\eta < \Theta$, then $\beta_\Theta \geq 1$.) Equation (30) is applied in Part 2 to a problem in which a special trial function is used which generates the Schwinger integral variational principle.

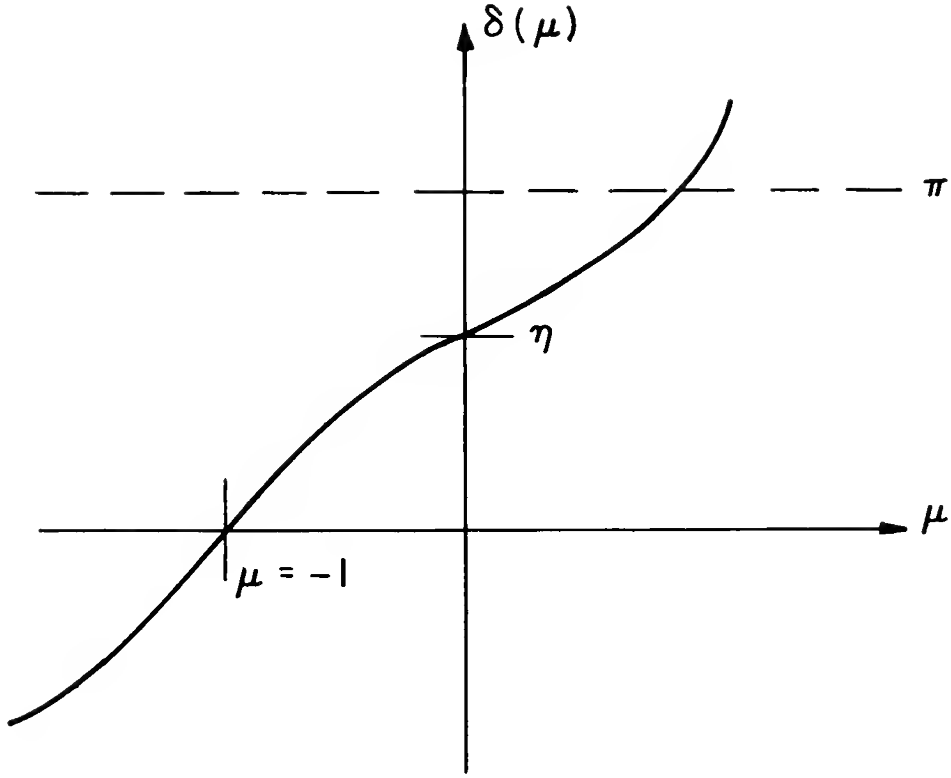

Figure 3

Determination of the exact value of β_θ assuming $W > 0$, $\rho = W$, $\theta = 0$ and $\eta < \pi$. In this case, β_0 is given exactly by $\beta_0 = 1$.

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14. Some further discussion on completeness is contained in reference 9.

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